

Supporting Information

Structure and Stability of Tube and Cage $\text{Ge}_{60}\text{H}_{60}$

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1. Calculation details for $\text{Ge}_{60}\text{H}_{60}$, Ge_6H_6 at GGA-PAW level by VASP.

We performed plane-wave-based, periodic DFT calculations with the Vienna ab-initio simulation package (VASP). The all-electron (frozen core) Projector Augmented Wave (PAW) DFT method was employed. The GGA of PW91 was utilized for the exchange-correlation functional. All the calculations are performed in a simple cubic supercell of $35\text{\AA}\times 35\text{\AA}\times 35\text{\AA}$ with one k-point. Other parameters are set to default value in VASP.

2. Calculation details for Ge_6H_6 at B3LYP/DZP level by the Amsterdam Density Functional (ADF) package.

The calculations are performed with B3LYP hybrid functional method. The basis set is standard ADF all election double-zeta slater orbitals with polarization functions (DZP). The zero-order regular approximation (ZORA) is adopted to account for the scalar relativistic effect for Germanium. Other parameters are set to default value in ADF.

3. Isomers considered to find the most stable endo isomers

(Energies (a.u.) are calculated at HF/Lan12dz; Index numbers of endo Ge atoms are based on isomer **1** for cage isomers, and on isomer **6** for tube isomers)

3.1 Cage isomers of $\text{H}_8@ \text{Ge}_{60}\text{H}_{52}$ (27 possibilities considered)

Isomer	Index of endo Ge atoms	Symmetry	Energy
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c-8-1 (isomer 2)	1,15,18,22,40,44,47,56	D_2	-263.1690843
c-8-2	1,14,17,22,41,46,48,52	C_1	-263.1652584
c-8-3	1,15,22,29,34,37,50,58	C_i	-263.1639404
c-8-4	1,15,22,27,34,41,49,58	C_1	-263.1636111
c-8-5	1,13,18,21,26,42,49,58	C_1	-263.1618894
c-8-6	1,9,13,30,35,48,51,58	C_i	-263.1614933
c-8-7	1,9,21,23,36,38,51,58	C_i	-263.1606592
c-8-8	1,14,16,22,37,41,49,58	C_i	-263.1604817
c-8-9	1,9,14,22,37,39,53,60	C_1	-263.1601998
c-8-10	1,17,29,34,36,42,50,54	C_1	-263.1600769
c-8-11	1,8,26,31,33,38,55,58	C_1	-263.1588755
c-8-12	1,8,27,30,35,42,55,58	C_1	-263.1588368
c-8-13	1,15,22,29,34,37,53,55	C_1	-263.1587466
c-8-14	1,8,21,33,39,45,47,51	C_1	-263.1586507
c-8-15	1,9,13,21,28,43,45,59	C_1	-263.1580555
c-8-16	1,9,14,21,39,44,54,56	C_1	-263.1567778
c-8-17	1,13,21,26,38,45,51,59	C_1	-263.1567339
c-8-18	2,9,20,31,37,43,45,58	C_2	-263.156232
c-8-19	1,18,21,25,33,39,46,57	D_2	-263.1555521
c-8-20	1,13,26,30,32,38,45,59	D_2	-263.1555518
c-8-21	1,8,18,26,32,50,52,59	D_2	-263.1555446
c-8-22	4,14,27,30,32,35,49,56	C_{2h}	-263.1549534
c-8-23	1,9,13,25,40,48,51,58	C_{2h}	-263.1549458
c-8-24	1,13,27,30,32,35,48,58	C_{2h}	-263.1549412
c-8-25	1,8,18,21,35,48,51,58	C_2	-263.1541772
c-8-26	1,13,16,18,31,43,48,58	C_2	-263.1539975
c-8-27	1,13,18,26,31,43,48,58	C_i	-263.1537881

3.2 Cage isomers of $H_{10}@Ge_{60}H_{50}$ (25 possibilities considered)

Isomer	Index of endo Ge atoms	Symmetry	Energy
c-10-1 (isomer 3)	1,13,15,17,21,29,42,44,46,55	C_2	-263.1805451
c-10-2	1,8,17,29,32,34,36,50,54,57	C_2	-263.1804826
c-10-3	1,9,14,22,30,35,37,49,51,58	C_5	-263.1790446
c-10-4	1,14,16,18,22,30,44,47,49,56	C_2	-263.1780748
c-10-5	1,14,16,18,22,30,44,46,49,51	C_1	-263.1780493
c-10-6	1,13,16,18,21,39,42,44,47,60	C_2	-263.1769679
c-10-7	1,13,15,18,21,39,42,44,46,60	C_1	-263.1767251
c-10-8	1,9,14,22,28,30,35,43,47,60	C_1	-263.176478
c-10-9	1,15,17,29,32,34,36,50,54,57	C_1	-263.1763229
c-10-10	1,8,18,23,26,31,39,45,54,56	C_1	-263.1762035
c-10-11	1,9,13,21,25,29,37,42,53,60	C_1	-263.1751114

c-10-12	1,8,18,21,26,33,39,45,51,54	C_1	-263.1751005
c-10-13	1,9,13,25,29,31,37,43,55,58	C_2	-263.1744566
c-10-14	1,8,12,17,34,36,39,41,54,57	C_1	-263.1744117
c-10-15	1,8,18,21,23,35,39,47,52,60	C_2	-263.1737042
c-10-16	1,8,23,27,29,31,35,52,54,55	C_1	-263.1725776
c-10-17	1,9,12,24,30,36,38,43,55,58	C_1	-263.1723429
c-10-18	1,8,17,19,21,23,44,47,49,56	C_1	-263.1715674
c-10-19	1,9,13,25,30,32,37,49,53,56	D_5	-263.170887
c-10-20	1,12,15,17,31,33,45,47,49,56	C_1	-263.1702319
c-10-21	1,13,15,17,29,34,36,50,54,57	C_1	-263.1688398
c-10-22	1,9,12,14,28,33,36,41,54,57	C_1	-263.1684244
c-10-23	1,9,13,25,30,32,45,47,49,56	C_1	-263.1654024
c-10-24	1,10,13,15,26,30,32,38,45,59	C_2	-263.1550881
c-10-25	3,13,16,29,30,34,35,41,48,60	D_{5d}	-263.1442052

3.3 Cage isomers of $H_{12}@Ge_{60}H_{48}$ (16 possibilities considered)

Isomer	Index of endo Ge atoms	Symmetry	Energy
c-12-1 (Isomer 4)	1,13,15,17,21,29,34,36,42,48,50,58	C_i	- 263.1792221
c-12-2	1,9,12,14,28,30,33,35,47,51,55,58	C_2	-263.179173
c-12-3	1,8,9,12,28,30,31,33,35,47,55,57	C_1	- 263.1778812
c-12-4	1,12,14,16,18,30,33,37,41,45,49,57	C_1	- 263.1746698
c-12-5	1,9,13,15,28,30,32,36,44,54,55,56	C_2	- 263.1686134
c-12-6	1,9,12,14,19,31,35,38,43,46,55,58	C_1	- 263.1684936
c-12-7	1,8,13,18,21,26,34,38,39,42,53,60	C_2	- 263.1672774
c-12-8	4,7,15,19,21,26,33,38,45,50,51,59	C_2	- 263.1671479
c-12-9	1,8,12,17,29,32,34,36,50,53,54,57	C_1	- 263.1652023
c-12-10	1,8,10,13,17,21,34,36,38,42,55,58	C_1	- 263.1650524

c-12-11	1,10,13,15,26,30,32,38,43,45,55,59	D_2	- 263.1545336
c-12-12	1,7,9,18,21,24,33,36,39,41,54,57	C_1	- 263.1542738
c-12-13	1,7,11,15,17,29,34,42,47,50,53,59	C_3	- 263.1532825
c-12-14	1,7,9,21,25,28,33,40,46,51,54,57	C_1	- 263.1531999
c-12-15	1,7,15,18,27,30,32,35,39,43,54,58	C_1	- 263.1386309
c-12-16	2,4,11,18,29,30,34,35,43,46,56,59	D_{3d}	- 263.1201225

3.4 Cage isomers of $H_{14}@Ge_{60}H_{46}$ (11 possibilities considered)

Isomer	Index of endo Ge atoms	Symmetry	Energy
c-14-1 (Isomer 5)	1,4,13,15,21,27,29,32,34,36,48,50,56,58	C_i	- 263.1589661
c-14-2	1,8,12,17,29,30,32,34,36,38,50,53,54,57	C_1	- 263.1519854
c-14-3	5,13,16,17,20,32,34,35,38,39,46,50,56,59	C_1	- 263.1487539
c-14-4	4,7,14,15,19,21,26,33,38,39,45,50,51,59	C_2	- 263.1451769
c-14-5	1,9,18,19,21,22,24,36,37,39,43,44,51,58	C_i	-263.143949
c-14-6	1,4,10,13,15,26,30,32,38,43,45,51,55,59	C_2	- 263.1424961
c-14-7	1,8,12,23,24,26,30,38,39,41,42,44,46,59	C_1	- 263.1417251
c-14-8	1,8,9,19,25,27,28,32,33,40,44,51,55,58	C_i	- 263.1346536
c-14-9	1,7,8,10,16,21,23,36,38,41,52,54,55,58	C_i	- 263.1222571

c-14-10	1,8,11,16,22,24,28,33,37,39,41,46,55,58	C_i	- 263.1118476
c-14-11	1,7,10,14,17,21,34,36,37,45,50,51,54,57	C_1	- 263.1118057

3.5 Cage isomers of $H_{16}@Ge_{60}H_{44}$ (10 possibilities considered)

Isomer	Index of endo Ge atoms	Symm.	Energy
c-16-1	1,8,12,17,19,23,25,26,31,38,40,42,44,47,55,58	C_i	- 263.1440637
c-16-2	1,3,12,13,17,19,25,26,31,33,40,44,47,49,51,58	C_1	- 263.1387804
c-16-3	3,5,13,16,17,20,21,22,34,35,38,39,46,50,56,59	C_1	- 263.1343264
c-16-4	1,7,8,9,19,25,27,28,32,33,40,44,51,54,55,58	C_i	- 263.1339197
c-16-5	1,3,10,12,16,23,24,30,36,37,39,41,42,48,52,59	C_1	- 263.1310155
c-16-6	3,5,13,17,20,21,22,29,34,36,37,45,48,50,56,57	C_1	- 263.1195972
c-16-7	1,4,8,12,20,25,27,28,31,33,40,44,48,51,57,59	C_1	- 263.1162663
c-16-8	1,9,10,12,24,27,30,32,33,35,38,39,41,46,52,58	C_2	-263.11608
c-16-9	1,4,8,10,22,24,26,30,31,35,37,39,52,55,56,58	C_i	- 263.1072031
c-16-10	2,7,16,19,25,26,29,30,31,34,35,40,41,44,54,59	C_{2v}	- 263.0361387

3.6 Tube isomers of $H_2@Ge_{60}H_{58}$ (24 possibilities considered)

Isomer	Index of endo Ge atoms	Symmetry	Energy
t-2-1 (Isomer 7)	21,38	C_{2h}	- 263.1577393
t-2-2	30,32	C_{2h}	-

			263.1567782
t-2-3	23,37	C_2	-263.156076
t-2-4	16,40	C_s	- 263.1552884
t-2-5	22,38	C_2	- 263.1547554
t-2-6	25,36	C_2	- 263.1546228
t-2-7	19,33	C_s	- 263.1543295
t-2-8	18,44	C_{2h}	- 263.1542923
t-2-9	18,42	C_2	- 263.1541368
t-2-10	25,30	C_s	- 263.1538044
t-2-11	19,41	C_2	- 263.1535953
t-2-12	16,41	C_2	- 263.1535773
t-2-13	20,29	C_1	- 263.1510601
t-2-14	29,32	C_2	- 263.1478163
t-2-15	27,33	C_2	- 263.1476888
t-2-16	11,40	C_s	- 263.1461399
t-2-17	17,46	C_1	- 263.1450421
t-2-18	35,39	C_1	- 263.1437679

t-2-19	11,16	C_s	- 263.1360311
t-2-20	13,47	C_2	- 263.1359103
t-2-21	14,50	C_{2h}	- 263.1358689
t-2-22	14,46	C_2	- 263.1358575
t-2-23	12,46	C_2	- 263.1356989
t-2-24	8,53	C_{2h}	- 263.1102392

3.7 Tube isomers of $H_4@Ge_{60}H_{56}$ (47 possibilities considered)

Isomer	Index of endo Ge atoms	Symmetry	Energy
t-4-1 (Isomer 8)	18,25,37,44	C_{2h}	- 263.1786562
t-4-2	18,30,32,44	C_{2h}	- 263.1781339
t-4-3	16,23,39,41	C_2	- 263.1767503
t-4-4	23,30,32,44	C_1	- 263.1742315
t-4-5	20,26,33,41	C_i	- 263.1724439
t-4-6	25,28,35,37	C_i	- 263.1715877
t-4-7	20,29,31,41	C_i	- 263.1697265
t-4-8	16,28,34,41	C_2	- 263.1686728
t-4-9	16,26,33,43	C_2	-

			263.1682236
t-4-10	22,24,36,38	C_2	- 263.1652584
t-4-11	16,29,35,43	C_2	-263.164634
t-4-12	18,29,32,43	C_2	- 263.1643077
t-4-13	22,25,41,44	C_s	- 263.1640568
t-4-14	16,18,41,44	C_2	- 263.1635312
t-4-15	18,20,41,44	C_{2h}	- 263.1634016
t-4-16	21,29,35,38	C_2	- 263.1633892
t-4-17	16,19,41,43	C_2	- 263.1631937
t-4-18	13,25,37,49	C_{2h}	- 263.1629488
t-4-19	27,30,41,44	C_s	- 263.1626352
t-4-20	20,21,38,41	C_i	- 263.1613768
t-4-21	16,24,38,41	C_2	- 263.1611744
t-4-22	16,22,40,41	C_2	- 263.1606926
t-4-23	13,30,32,49	C_{2h}	-263.160467
t-4-24	20,29,35,44	C_2	- 263.1602412
t-4-25	13,27,34,48	C_2	- 263.1595878
t-4-26	12,26,33,48	C_i	-

			263.1594757
t-4-27	13,25,36,48	C_2	- 263.1586609
t-4-28	12,28,35,48	C_i	- 263.1576453
t-4-29	12,23,40,48	C_i	- 263.1571791
t-4-30	13,21,40,48	C_2	- 263.1565566
t-4-31	12,20,34,38	C_1	- 263.1559718
t-4-32	13,24,37,48	C_2	- 263.1553294
t-4-33	12,19,45,48	C_i	- 263.1550656
t-4-34	15,18,44,46	C_i	- 263.1550032
t-4-35	13,16,42,50	C_2	- 263.1548594
t-4-36	13,20,41,48	C_2	- 263.1548579
t-4-37	13,16,45,48	C_2	- 263.1542862
t-4-38	11,16,35,40	C_s	- 263.1529768
t-4-39	20,29,38,47	C_1	- 263.1526472
t-4-40	13,30,31,48	C_2	- 263.1500018
t-4-41	13,29,32,48	C_2	- 263.1498069
t-4-42	28,35,47,54	C_s	-

			263.1457686
t-4-43	11,16,23,28	C_s	- 263.1394981
t-4-44	11,16,42,47	C_{2h}	- 263.1391508
t-4-45	13,15,46,48	C_2	- 263.1322999
t-4-46	13,15,46,49	C_{2h}	- 263.1322751
t-4-47	11,13,48,50	C_2	- 263.1320962

3.8 Tube isomers of $H_6@Ge_{60}H_{54}$ (31 possibilities considered)

Isomer	Index of endo Ge atoms	Symmetry	Energy
t-6-1 (Isomer 9)	17,19,30,32,43,45	C_{2h}	- 263.1825929
t-6-2	17,19,29,31,41,43	C_2	- 263.1788165
t-6-3	12,20,27,34,41,48	C_i	- 263.1783308
t-6-4	12,19,26,33,45,48	C_i	- 263.1783292
t-6-5	17,19,28,35,43,45	C_i	- 263.1783277
t-6-6	19,21,29,35,38,45	C_2	-263.178124
t-6-7	11,19,26,33,45,48	C_2	-263.178044
t-6-8	14,16,28,35,42,50	C_i	- 263.1779964
t-6-9	13,25,28,35,37,49	C_i	-263.176137
t-6-10	16,18,29,32,35,43	C_s	- 263.1740517
t-6-11	12,19,27,34,45,48	C_i	-263.174024
t-6-12	12,19,30,32,45,48	C_i	-

			263.1726705
t-6-13	21,23,30,32,44,47	C_1	- 263.1723823
t-6-14	14,16,26,33,42,50	C_i	- 263.1709021
t-6-15	18,21,28,35,38,44	C_i	- 263.1699571
t-6-16	14,16,26,33,43,50	C_2	- 263.1696125
t-6-17	17,20,27,30,36,39	C_1	- 263.1695839
t-6-18	12,19,26,34,41,48	C_2	- 263.1693158
t-6-19	12,23,26,34,37,48	C_2	- 263.1690996
t-6-20	12,20,26,34,45,48	C_2	- 263.1654504
t-6-21	20,21,29,35,38,44	C_2	- 263.1634879
t-6-22	7,19,26,33,45,52	C_{2h}	- 263.1569515
t-6-23	12,14,26,33,48,50	C_i	- 263.1562123
t-6-24	12,14,29,31,48,50	C_i	- 263.1561797
t-6-25	12,14,29,31,46,48	C_2	-263.155884
t-6-26	12,14,25,37,48,50	C_{2h}	- 263.1536131
t-6-27	10,18,25,37,44,52	C_2	- 263.1508126
t-6-28	12,14,27,33,46,48	C_2	- 263.1469341

t-6-29	12,14,26,34,46,48	C_2	-263.146579
t-6-30	26,27,29,41,43,45	C_s	263.1461925
t-6-31	6,13,30,32,49,51	C_{2h}	263.1345971

3.9 Tube isomers of $H_8@Ge_{60}H_{52}$ (42 possibilities considered)

Isomer	Index of endo Ge atoms	Symmetry	Energy
t-8-1 (Isomer 10)	17,19,25,28,35,37,43,45	C_i	263.1792573
t-8-2	17,19,25,27,33,40,41,43	C_2	263.1777795
t-8-3	12,19,25,27,33,40,41,48	C_2	263.1743184
t-8-4	13,20,22,29,31,38,45,47	C_2	263.1711032
t-8-5	15,17,23,30,33,36,42,49	C_1	263.1706587
t-8-6	11,17,19,30,32,43,45,47	C_i	-263.170634
t-8-7	12,19,21,29,35,38,45,47	C_2	263.1700831
t-8-8	15,18,21,28,31,34,45,48	C_1	263.1685577
t-8-9	13,15,21,23,30,32,44,47	C_1	263.1684884
t-8-10	13,15,21,29,31,38,46,49	C_i	263.1679156
t-8-11	15,17,23,25,37,40,43,46	C_i	263.1671361
t-8-12	12,14,25,27,33,40,46,48	C_2	-263.166012
t-8-13	12,15,23,26,32,34,41,48	C_1	263.1657845
t-8-14	17,20,28,30,31,34,42,44	C_2	263.1632197

t-8-15	17,19,25,28,32,40,41,43	C_2	- 263.1628761
t-8-16	13,15,21,29,35,38,46,49	C_2	- 263.1605266
t-8-17	12,14,16,28,35,42,48,50	C_i	- 263.1602009
t-8-18	13,17,19,30,32,43,45,49	C_{2h}	- 263.1598098
t-8-19	12,14,16,29,31,42,48,50	C_i	-263.159222
t-8-20	12,14,20,26,33,41,48,50	C_i	- 263.1592026
t-8-21	11,18,23,25,37,40,43,46	C_1	- 263.1553027
t-8-22	12,14,25,29,31,40,46,48	C_2	- 263.1520636
t-8-23	12,18,25,26,34,40,42,48	C_2	- 263.1518014
t-8-24	12,14,25,30,32,37,48,50	C_{2h}	- 263.1495933
t-8-25	11,13,20,26,28,39,40,46	C_1	-263.147646
t-8-26	11,18,27,28,30,39,40,46	C_1	- 263.1470853
t-8-27	9,15,17,29,31,43,50,51	C_2	- 263.1456523
t-8-28	9,15,17,29,31,43,46,54	C_i	- 263.1454686
t-8-29	12,14,27,30,33,35,46,48	C_2	- 263.1408746
t-8-30	18,19,25,35,37,38,49,50	C_1	- 263.1359749
t-8-31	12,17,24,29,31,36,43,48	C_{2h}	- 263.1337591

t-8-32	12,14,27,28,34,35,48,50	C_{2h}	- 263.1296224
t-8-33	22,25,27,30,33,38,45,50	C_s	- 263.1262795
t-8-34	14,19,21,26,32,37,44,49	C_2	- 263.1256153
t-8-35	12,17,24,29,35,40,42,47	C_2	- 263.1256008
t-8-36	14,19,25,30,32,37,45,50	C_i	- 263.1156919
t-8-37	15,20,23,28,35,40,41,46	C_i	- 263.1156908
t-8-38	12,17,23,28,35,40,41,46	C_2	- 263.1153683
t-8-39	14,19,25,30,32,37,43,48	C_2	- 263.1152807
t-8-40	12,14,16,20,41,42,48,50	C_{2h}	-263.099116
t-8-41	12,14,17,19,42,45,47,50	C_2	- 263.0884209
t-8-42	12,14,17,19,43,45,48,50	C_{2h}	-263.088347

3.10 Tube isomers of $H_{10}@Ge_{60}H_{50}$ (21 possibilities considered)

Isomer	Index of endo Ge atoms	Symmetry	Energy
t-10-1	11,14,22,24,26,33,36,39,47,50	C_i	- 263.1611925
t-10-2	11,13,22,24,26,33,36,39,47,50	C_1	- 263.1609461
t-10-3	11,17,19,25,26,33,37,43,45,47	C_i	- 263.1601153
t-10-4	12,14,20,22,26,33,39,41,48,50	C_i	-263.158664
t-10-5	12,15,16,23,30,32,40,42,46,48	C_i	- 263.1547112
t-10-6	14,17,20,28,30,31,42,44,48,50	C_1	- 263.1540193

t-10-7	11,14,23,25,27,34,37,40,47,50	C_i	- 263.1528319
t-10-8	12,15,18,21,30,33,36,39,42,50	C_1	- 263.1521318
t-10-9	12,15,22,25,29,31,38,40,48,50	C_2	- 263.1521233
t-10-10	16,18,24,26,27,33,34,36,42,44	C_{2h}	- 263.1519518
t-10-11	11,14,17,25,27,33,40,43,46,49	C_2	- 263.1502046
t-10-12	17,19,25,28,29,31,35,37,43,45	C_i	- 263.1465999
t-10-13	12,15,16,23,27,34,40,42,46,48	C_i	- 263.1459875
t-10-14	12,15,16,23,27,34,40,42,46,48	C_i	- 263.1459809
t-10-15	11,14,20,22,30,33,39,41,47,50	C_i	- 263.1457947
t-10-16	12,15,16,23,29,31,40,42,46,48	C_i	- 263.1457942
t-10-17	13,15,22,25,29,36,39,42,46,49	C_1	- 263.1424006
t-10-18	12,15,16,18,26,28,36,38,46,48	C_1	- 263.1423102
t-10-19	7,14,20,22,26,33,39,41,50,52	C_i	- 263.1386619
t-10-20	13,17,19,25,30,31,33,37,44,49	C_s	- 263.1362872
t-10-21	1,12,14,23,26,32,39,47,50,58	C_1	- 263.1001558

4 The Coordinates and electronic energies of isomer 1-10 at B3LYP/cc-pVDZ

Isomer 1, HF=-124658.5414754 a.u.

Ge -0.4074068722 -5.2650099173 3.1725029718
Ge 1.3061819706 -4.0200147473 4.4815683623
Ge 3.4242942661 -4.0200147472 3.1725029719
Ge 3.0197708138 -5.2650099172 1.0543906765
Ge 0.6516492756 -6.0344592482 1.0543906765
Ge -2.7650960991 -4.4989502500 3.1725029716
Ge 0.6545326951 -2.0144445005 5.7848669129
Ge 4.8814263431 -2.0144445004 3.1725029719
Ge 4.0741614901 -4.4989502498 -1.0543906759
Ge -0.6516492750 -6.0344592483 -1.0543906761
Ge -3.4196287946 -2.4845057493 4.4815683621
Ge -1.7135888431 -1.2449951698 5.7848669128
Ge 2.1181122951 0.0000000003 5.7848669129
Ge 4.2268936477 0.0000000004 4.4815683623
Ge 5.9404824908 -1.2449951696 1.0543906765
Ge 5.5377410901 -2.4845057490 -1.0543906760
Ge 2.7650960996 -4.4989502499 -3.1725029714
Ge 0.4074068727 -5.2650099175 -3.1725029714
Ge -3.0197708132 -5.2650099176 -1.0543906762
Ge -4.0741614896 -4.4989502502 1.0543906762
Ge -5.1332176375 -1.2395105795 3.1725029715
Ge -1.7135888432 1.2449951700 5.7848669127
Ge 0.6545326949 2.0144445010 5.7848669128
Ge 4.8814263429 2.0144445011 3.1725029717
Ge 5.9404824907 1.2449951703 1.0543906764
Ge 5.1332176377 -1.2395105791 -3.1725029714
Ge 3.4196287948 -2.4845057492 -4.4815683619
Ge -1.3061819702 -4.0200147477 -4.4815683621
Ge -3.4242942656 -4.0200147478 -3.1725029716
Ge -5.5377410898 -2.4845057495 1.0543906761
Ge -5.1332176377 1.2395105791 3.1725029714
Ge -3.4196287948 2.4845057492 4.4815683619
Ge 1.3061819702 4.0200147477 4.4815683621
Ge 3.4242942656 4.0200147478 3.1725029716
Ge 5.5377410898 2.4845057495 -1.0543906761
Ge 5.1332176375 1.2395105795 -3.1725029715
Ge 1.7135888432 -1.2449951700 -5.7848669127
Ge -0.6545326949 -2.0144445010 -5.7848669128
Ge -4.8814263429 -2.0144445011 -3.1725029717
Ge -5.9404824907 -1.2449951703 -1.0543906764
Ge -5.5377410901 2.4845057490 1.0543906760
Ge -2.7650960996 4.4989502499 3.1725029714
Ge -0.4074068727 5.2650099175 3.1725029714

Ge 3.0197708132 5.2650099176 1.0543906762
Ge 4.0741614896 4.4989502502 -1.0543906762
Ge 3.4196287946 2.4845057493 -4.4815683621
Ge 1.7135888431 1.2449951698 -5.7848669128
Ge -2.1181122951 -0.0000000003 -5.7848669129
Ge -4.2268936477 -0.0000000004 -4.4815683623
Ge -5.9404824908 1.2449951696 -1.0543906765
Ge -4.0741614901 4.4989502498 1.0543906759
Ge 0.6516492750 6.0344592483 1.0543906761
Ge 2.7650960991 4.4989502500 -3.1725029716
Ge -0.6545326951 2.0144445005 -5.7848669129
Ge -4.8814263431 2.0144445004 -3.1725029719
Ge -3.0197708138 5.2650099172 -1.0543906765
Ge -0.6516492756 6.0344592482 -1.0543906765
Ge 0.4074068722 5.2650099173 -3.1725029718
Ge -1.3061819706 4.0200147473 -4.4815683623
Ge -3.4242942661 4.0200147472 -3.1725029719
H -0.5228094371 -6.5947391406 3.9761381275
H 1.6336820536 -5.0279563610 5.6235510336
H 4.2992521293 -5.0279563609 3.9761381276
H 3.7901735447 -6.5947391404 1.3105680521
H 0.8099756009 -7.5630641512 1.3105680520
H -3.4533286899 -5.6425557153 3.9761381273
H 0.8237064529 -2.5351077898 7.2435022346
H 6.1104126320 -2.5351077896 3.9761381276
H 5.1007415965 -5.6425557150 -1.3105680513
H -0.8099756001 -7.5630641514 -1.3105680515
H -4.2770351431 -3.1074479253 5.6235510333
H -2.1564914910 -1.5667827793 7.2435022344
H 2.6655700753 0.0000000004 7.2435022346
H 5.2867061788 0.0000000005 5.6235510336
H 7.4431976699 -1.5667827789 1.3105680520
H 6.9426052189 -3.1074479249 -1.3105680514
H 3.4533286905 -5.6425557152 -3.9761381270
H 0.5228094378 -6.5947391408 -3.9761381271
H -3.7901735440 -6.5947391409 -1.3105680517
H -5.1007415959 -5.6425557155 1.3105680517
H -6.4335266340 -1.5406651461 3.9761381271
H -2.1564914912 1.5667827795 7.2435022343
H 0.8237064526 2.5351077903 7.2435022344
H 6.1104126318 2.5351077905 3.9761381275
H 7.4431976697 1.5667827798 1.3105680520
H 6.4335266342 -1.5406651456 -3.9761381270
H 4.2770351435 -3.1074479252 -5.6235510331

H -1.6336820531 -5.0279563615 -5.6235510333
H -4.2992521287 -5.0279563616 -3.9761381273
H -6.9426052186 -3.1074479256 1.3105680515
H -6.4335266342 1.5406651456 3.9761381270
H -4.2770351435 3.1074479252 5.6235510331
H 1.6336820531 5.0279563615 5.6235510333
H 4.2992521287 5.0279563616 3.9761381273
H 6.9426052186 3.1074479256 -1.3105680515
H 6.4335266340 1.5406651461 -3.9761381271
H 2.1564914912 -1.5667827795 -7.2435022343
H -0.8237064526 -2.5351077903 -7.2435022344
H -6.1104126318 -2.5351077905 -3.9761381275
H -7.4431976697 -1.5667827798 -1.3105680520
H -6.9426052189 3.1074479249 1.3105680514
H -3.4533286905 5.6425557152 3.9761381270
H -0.5228094378 6.5947391408 3.9761381271
H 3.7901735440 6.5947391409 1.3105680517
H 5.1007415959 5.6425557155 -1.3105680517
H 4.2770351431 3.1074479253 -5.6235510333
H 2.1564914910 1.5667827793 -7.2435022344
H -2.6655700753 -0.0000000004 -7.2435022346
H -5.2867061788 -0.0000000005 -5.6235510336
H -7.4431976699 1.5667827789 -1.3105680520
H -5.1007415965 5.6425557150 1.3105680513
H 0.8099756001 7.5630641514 1.3105680515
H 3.4533286899 5.6425557153 -3.9761381273
H -0.8237064529 2.5351077898 -7.2435022346
H -6.1104126320 2.5351077896 -3.9761381276
H -3.7901735447 6.5947391404 -1.3105680521
H -0.8099756009 7.5630641512 -1.3105680520
H 0.5228094371 6.5947391406 -3.9761381275
H -1.6336820536 5.0279563610 -5.6235510336
H -4.2992521293 5.0279563609 -3.9761381276

Isomer 2, HF=-124658.6580708 a.u.

Ge 1.9222720079 1.5740978758 3.9991925799
Ge 4.3504796210 1.2288131528 3.8726259988
Ge 4.5706649036 -1.2371210017 4.0910511101
Ge 2.5323048212 -2.0499330260 5.3520175602
Ge 1.2283745972 0.0425328366 5.7859809713
Ge 1.1964658304 3.8784032159 4.3918936415
Ge 5.3820721225 2.4828064960 2.0029791111
Ge 4.9677747157 -2.3689381970 1.9340645446
Ge 1.2793565411 -4.0701070396 4.5380368267

Ge -1.2283745972 -0.0425328366 5.7859809713
Ge 2.0303681880 5.3159088341 2.5396125084
Ge 3.8257867772 4.2647715055 1.1766508172
Ge 6.1435868250 1.2432587772 -0.0481106635
Ge 6.1435868250 -1.2432587772 0.0481106635
Ge 2.9460294704 -3.3110845554 0.9094645350
Ge 1.9424309236 -5.0172533124 2.3408754387
Ge -1.1964658304 -3.8784032159 4.3918936415
Ge -1.9222720079 -1.5740978758 3.9991925799
Ge -2.5323048212 2.0499330260 5.3520175602
Ge -1.2793565411 4.0701070396 4.5380368267
Ge 0.0193336849 6.1011879827 1.2564147545
Ge 2.9460294704 3.3110845554 -0.9094645350
Ge 4.9677747157 2.3689381970 -1.9340645446
Ge 5.3820721225 -2.4828064960 -2.0029791111
Ge 3.8257867772 -4.2647715055 -1.1766508172
Ge -0.0193336849 -6.1011879827 1.2564147545
Ge -2.0303681880 -5.3159088341 2.5396125084
Ge -4.3504796210 -1.2288131528 3.8726259988
Ge -4.5706649036 1.2371210017 4.0910511101
Ge -1.9424309236 5.0172533124 2.3408754387
Ge -0.0193336849 6.1011879827 -1.2564147545
Ge 1.9424309236 5.0172533124 -2.3408754387
Ge 4.5706649036 1.2371210017 -4.0910511101
Ge 4.3504796210 -1.2288131528 -3.8726259988
Ge 2.0303681880 -5.3159088341 -2.5396125084
Ge 0.0193336849 -6.1011879827 -1.2564147545
Ge -3.8257867772 -4.2647715055 1.1766508172
Ge -5.3820721225 -2.4828064960 2.0029791111
Ge -4.9677747157 2.3689381970 1.9340645446
Ge -2.9460294704 3.3110845554 0.9094645350
Ge -2.0303681880 5.3159088341 -2.5396125084
Ge 1.2793565411 4.0701070396 -4.5380368267
Ge 2.5323048212 2.0499330260 -5.3520175602
Ge 1.9222720079 -1.5740978758 -3.9991925799
Ge 1.1964658304 -3.8784032159 -4.3918936415
Ge -1.9424309236 -5.0172533124 -2.3408754387
Ge -2.9460294704 -3.3110845554 -0.9094645350
Ge -6.1435868250 -1.2432587772 -0.0481106635
Ge -6.1435868250 1.2432587772 0.0481106635
Ge -3.8257867772 4.2647715055 -1.1766508172
Ge -1.1964658304 3.8784032159 -4.3918936415
Ge 1.2283745972 -0.0425328366 -5.7859809713
Ge -1.2793565411 -4.0701070396 -4.5380368267

Ge -4.9677747157 -2.3689381970 -1.9340645446
Ge -5.3820721225 2.4828064960 -2.0029791111
Ge -1.9222720079 1.5740978758 -3.9991925799
Ge -1.2283745972 0.0425328366 -5.7859809713
Ge -2.5323048212 -2.0499330260 -5.3520175602
Ge -4.5706649036 -1.2371210017 -4.0910511101
Ge -4.3504796210 1.2288131528 -3.8726259988
H 1.2777361153 1.0852524953 2.6678324706
H 4.9362821508 1.8506211928 5.1746609414
H 5.7980710467 -1.5399385643 4.9999049413
H 3.0870607291 -2.5076242640 6.7349641298
H 1.7618561237 0.6286803083 7.1260195315
H 1.8349713133 4.3608879794 5.7243440016
H 6.6508615603 3.1741707462 2.5830301712
H 5.8481016345 -3.6156284320 2.2496117094
H 1.5798875713 -5.1585140512 5.6121208802
H -1.7618561237 -0.6286803083 7.1260195315
H 2.6437925806 6.5999761112 3.1731605914
H 4.7348455845 5.4419880956 0.7105627375
H 7.6521059221 1.6049717332 -0.1880389786
H 7.6521059221 -1.6049717332 0.1880389786
H 1.9119812605 -2.1898578387 0.6044120052
H 3.0320930727 -6.1020418830 2.5753101738
H -1.8349713133 -4.3608879794 5.7243440016
H -1.2777361153 -1.0852524953 2.6678324706
H -3.0870607291 2.5076242640 6.7349641298
H -1.5798875713 5.1585140512 5.6121208802
H -0.0866745554 7.6154206636 1.6118651914
H 1.9119812605 2.1898578387 -0.6044120052
H 5.8481016345 3.6156284320 -2.2496117094
H 6.6508615603 -3.1741707462 -2.5830301712
H 4.7348455846 -5.4419880956 -0.7105627375
H 0.0866745554 -7.6154206636 1.6118651914
H -2.6437925806 -6.5999761112 3.1731605914
H -4.9362821508 -1.8506211928 5.1746609414
H -5.7980710467 1.5399385643 4.9999049413
H -3.0320930727 6.1020418830 2.5753101738
H 0.0866745554 7.6154206636 -1.6118651914
H 3.0320930727 6.1020418830 -2.5753101738
H 5.7980710467 1.5399385643 -4.9999049413
H 4.9362821508 -1.8506211928 -5.1746609414
H 2.6437925806 -6.5999761112 -3.1731605914
H -0.0866745554 -7.6154206636 -1.6118651914
H -4.7348455845 -5.4419880956 0.7105627375

H -6.6508615603 -3.1741707462 2.5830301712
H -5.8481016345 3.6156284320 2.2496117094
H -1.9119812605 2.1898578387 0.6044120052
H -2.6437925806 6.5999761112 -3.1731605914
H 1.5798875713 5.1585140512 -5.6121208802
H 3.0870607291 2.5076242640 -6.7349641298
H 1.2777361153 -1.0852524953 -2.6678324706
H 1.8349713133 -4.3608879794 -5.7243440016
H -3.0320930727 -6.1020418830 -2.5753101738
H -1.9119812605 -2.1898578387 -0.6044120052
H -7.6521059221 -1.6049717332 -0.1880389786
H -7.6521059221 1.6049717332 0.1880389786
H -4.7348455846 5.4419880956 -0.7105627375
H -1.8349713133 4.3608879794 -5.7243440016
H 1.7618561237 -0.6286803083 -7.1260195315
H -1.5798875713 -5.1585140512 -5.6121208802
H -5.8481016345 -3.6156284320 -2.2496117094
H -6.6508615603 3.1741707462 -2.5830301712
H -1.2777361153 1.0852524953 -2.6678324706
H -1.7618561237 0.6286803083 -7.1260195315
H -3.0870607291 -2.5076242640 -6.7349641298
H -5.7980710467 -1.5399385643 -4.9999049413
H -4.9362821508 1.8506211928 -5.1746609414

Isomer 3, HF=-124658.6708298 a.u.

Ge -1.2092636957 2.2558762207 -4.0930584831
Ge 0.1623596596 1.2202886645 -5.8478269603
Ge 2.4618017550 2.0675398192 -5.3877334256
Ge 2.1414502665 4.2325159307 -4.1339246546
Ge -0.3398080959 4.5511195481 -3.9190572376
Ge -3.6185053304 1.9598017893 -4.4460666537
Ge -0.1623596596 -1.2202886645 -5.8478269603
Ge 4.0756409357 0.4845871759 -4.3453687467
Ge 3.3308380244 4.5873941125 -1.9786255713
Ge -1.4320021061 5.7759138242 -2.0473800711
Ge -4.0756409357 -0.4845871759 -4.3453687467
Ge -2.4618017550 -2.0675398192 -5.3877334256
Ge 1.2092636957 -2.2558762207 -4.0930584831
Ge 3.6185053304 -1.9598017893 -4.4460666537
Ge 4.3633791119 0.7789336778 -1.9172443118
Ge 5.1158364969 3.0181907563 -1.2598760348
Ge 1.8175914063 4.4539397912 -0.0391769345
Ge -0.0349636525 6.0576877690 0.0069655096
Ge -3.5411659440 4.6807670829 -1.2445887985

Ge -4.8653358339 3.0390121174 -2.5688526278
Ge -4.3633791119 -0.7789336778 -1.9172443118
Ge -2.1414502665 -4.2325159307 -4.1339246546
Ge 0.3398080959 -4.5511195481 -3.9190572376
Ge 4.8653358339 -3.0390121174 -2.5688526278
Ge 5.7640153956 -1.1296659129 -1.2167167310
Ge 5.2661897782 3.1485953814 1.2289014644
Ge 3.3117891638 4.5541047117 1.9221050072
Ge -1.4374800462 5.4403678766 1.9599664439
Ge -2.8928036938 3.7340225931 0.9388687943
Ge -5.7640153956 1.1296659129 -1.2167167310
Ge -5.1158364969 -3.0181907563 -1.2598760348
Ge -3.3308380244 -4.5873941125 -1.9786255713
Ge 1.4320021061 -5.7759138242 -2.0473800711
Ge 3.5411659440 -4.6807670829 -1.2445887985
Ge 6.0284042535 -1.1903185778 1.2557743853
Ge 5.3298236455 0.9409759087 2.3690348706
Ge 2.1276476824 4.2112419268 4.0833994686
Ge -0.3166234093 4.7315596336 4.0674322481
Ge -4.6967343414 2.9639224640 2.4071893018
Ge -6.0284042535 1.1903185778 1.2557743853
Ge -5.2661897782 -3.1485953814 1.2289014644
Ge -1.8175914063 -4.4539397912 -0.0391769345
Ge 0.0349636525 -6.0576877690 0.0069655096
Ge 2.8928036938 -3.7340225931 0.9388687943
Ge 4.6967343414 -2.9639224640 2.4071893018
Ge 3.1589150607 0.3604954141 3.3878566146
Ge 2.3778809127 1.9514298306 5.0705583002
Ge -1.4971598976 2.8923843763 5.3007525148
Ge -3.5421062263 1.8828274014 4.3186171128
Ge -5.3298236455 -0.9409759087 2.3690348706
Ge -3.3117891638 -4.5541047117 1.9221050072
Ge 1.4374800462 -5.4403678766 1.9599664439
Ge 3.5421062263 -1.8828274014 4.3186171128
Ge 0.2243048216 1.2377932261 6.0867766758
Ge -3.1589150607 -0.3604954141 3.3878566146
Ge -2.1276476824 -4.2112419268 4.0833994686
Ge 0.3166234093 -4.7315596336 4.0674322481
Ge 1.4971598976 -2.8923843763 5.3007525148
Ge -0.2243048216 -1.2377932261 6.0867766758
Ge -2.3778809127 -1.9514298306 5.0705583002
H -0.8694960735 1.5261834644 -2.7590210459
H -0.2763753867 1.8184076476 -7.2157717249
H 3.0958959297 2.4741975190 -6.7510818827

H 2.6595404191 5.3509227978 -5.0872478751
H -0.7875183491 5.2843169480 -5.2190319496
H -4.0369265302 2.5960305887 -5.8000257410
H 0.2763753867 -1.8184076476 -7.2157717249
H 5.4541061461 0.7735696866 -5.0098275715
H 3.9008342125 6.0352694727 -2.0272902847
H -1.8013788277 7.1902763690 -2.5835946559
H -5.4541061461 -0.7735696866 -5.0098275715
H -3.0958959297 -2.4741975190 -6.7510818827
H 0.8694960735 -1.5261834644 -2.7590210459
H 4.0369265302 -2.5960305887 -5.8000257410
H 2.9613685571 0.5870323867 -1.2639475254
H 6.4930139665 3.3352811794 -1.9044663773
H 1.1658723652 3.0390398436 -0.0626648258
H 0.5151004503 7.5084016269 0.0836873623
H -4.5224053226 5.8512826360 -0.9362020911
H -6.0774223522 3.8152889449 -3.1626599205
H -2.9613685571 -0.5870323867 -1.2639475254
H -2.6595404191 -5.3509227978 -5.0872478751
H 0.7875183491 -5.2843169480 -5.2190319496
H 6.0774223522 -3.8152889449 -3.1626599205
H 7.1877809825 -0.8554884403 -1.7878521226
H 6.5746201639 3.9011914816 1.6106286623
H 3.8490276467 6.0160002627 1.9740463601
H -2.3452704855 6.6438783787 2.3509018013
H -2.0081600114 2.4824480086 0.6571459999
H -7.1877809825 0.8554884403 -1.7878521226
H -6.4930139665 -3.3352811794 -1.9044663773
H -3.9008342125 -6.0352694727 -2.0272902847
H 1.8013788277 -7.1902763690 -2.5835946559
H 4.5224053226 -5.8512826360 -0.9362020911
H 7.5386677463 -1.4295540158 1.5493530061
H 6.3076060418 1.1174396820 3.5696835697
H 2.7544557018 5.2297381664 5.0820543821
H -0.4606017478 5.9635047712 5.0109901989
H -5.6064849702 4.1533627792 2.8198202682
H -7.5386677463 1.4295540158 1.5493530061
H -6.5746201639 -3.9011914816 1.6106286623
H -1.1658723652 -3.0390398436 -0.0626648258
H -0.5151004503 -7.5084016269 0.0836873623
H 2.0081600114 -2.4824480086 0.6571459999
H 5.6064849702 -4.1533627792 2.8198202682
H 2.0840360009 0.2616370278 2.2664669665
H 3.4547445371 2.0147329895 6.1899286484

H -1.9867158703 3.5710624918 6.6158510744
H -4.5353936970 1.7058923705 5.5046329552
H -6.3076060418 -1.1174396820 3.5696835697
H -3.8490276467 -6.0160002627 1.9740463601
H 2.3452704855 -6.6438783787 2.3509018013
H 4.5353936970 -1.7058923705 5.5046329552
H 0.3662322851 1.5533453915 7.6070473078
H -2.0840360009 -0.2616370278 2.2664669665
H -2.7544557018 -5.2297381664 5.0820543821
H 0.4606017478 -5.9635047712 5.0109901989
H 1.9867158703 -3.5710624918 6.6158510744
H -0.3662322851 -1.5533453915 7.6070473078
H -3.4547445371 -2.0147329895 6.1899286484

Isomer 4, HF=-124658.6710976 a.u.

Ge -0.3063500289 4.0855456894 2.4983555230
Ge 0.5982106948 5.8702075506 1.0727577918
Ge 3.0522910550 5.4034609389 1.0200302151
Ge 3.5272564330 4.1208593549 3.1441989082
Ge 1.3248044626 3.9115293780 4.3308461260
Ge -2.6434378896 4.4560101108 3.1385710016
Ge -0.6216464558 5.9623276044 -1.0688774756
Ge 4.0307871404 4.4353882395 -1.0599402346
Ge 4.7719204806 1.9657100098 3.0640427220
Ge 0.7545606046 2.0629145479 5.8985771736
Ge -4.0196267200 4.4299968115 1.0599087249
Ge -3.0647356613 5.4233957223 -1.0177627996
Ge 0.3007133976 4.2471404287 -2.5610236345
Ge 2.6774257238 4.4765134109 -3.1580321846
Ge 4.5091979932 2.0241042093 -0.8822170070
Ge 5.9202974429 1.2563280544 0.9780262857
Ge 3.3217028967 0.0206002474 3.5183068189
Ge 2.1863090064 0.0267604107 5.6911027140
Ge -1.6171186402 1.2500481200 5.7141671189
Ge -3.4122774684 2.5860247691 4.6088237534
Ge -4.4523766932 2.0129518422 0.8813379592
Ge -3.5373964467 4.1250819859 -3.1324830198
Ge -1.3619514487 3.9475911337 -4.3591243008
Ge 3.3218962453 2.4584305497 -4.5014773007
Ge 5.0209766259 1.2360421476 -3.1715313501
Ge 5.8897430568 -1.2489429583 0.9665514774
Ge 4.7468243747 -1.9484501314 3.0592699520
Ge 0.6975689824 -1.9531315838 5.6933235110
Ge -1.3506069270 -0.9880986913 4.6947125906

Ge -4.9690007889 1.2489474464 3.1782745601
Ge -5.8897430568 1.2489429583 -0.9665514774
Ge -4.7468243747 1.9484501314 -3.0592699520
Ge -0.6975689824 1.9531315838 -5.6933235110
Ge 1.3506069270 0.9880986913 -4.6947125906
Ge 4.9690007889 -1.2489474464 -3.1782745601
Ge 4.4523766932 -2.0129518422 -0.8813379592
Ge 3.5373964467 -4.1250819859 3.1324830198
Ge 1.3619514487 -3.9475911337 4.3591243008
Ge -3.3218962453 -2.4584305497 4.5014773007
Ge -5.0209766259 -1.2360421476 3.1715313501
Ge -5.9202974429 -1.2563280544 -0.9780262857
Ge -3.3217028967 -0.0206002474 -3.5183068189
Ge -2.1863090064 -0.0267604107 -5.6911027140
Ge 1.6171186402 -1.2500481200 -5.7141671189
Ge 3.4122774684 -2.5860247691 -4.6088237534
Ge 4.0196267200 -4.4299968115 -1.0599087249
Ge 3.0647356613 -5.4233957223 1.0177627996
Ge -0.3007133976 -4.2471404287 2.5610236345
Ge -2.6774257238 -4.4765134109 3.1580321846
Ge -4.5091979932 -2.0241042093 0.8822170070
Ge -4.7719204806 -1.9657100098 -3.0640427220
Ge -0.7545606046 -2.0629145479 -5.8985771736
Ge 2.6434378896 -4.4560101108 -3.1385710016
Ge 0.6216464558 -5.9623276044 1.0688774756
Ge -4.0307871404 -4.4353882395 1.0599402346
Ge -3.5272564330 -4.1208593549 -3.1441989082
Ge -1.3248044626 -3.9115293780 -4.3308461260
Ge 0.3063500289 -4.0855456894 -2.4983555230
Ge -0.5982106948 -5.8702075506 -1.0727577918
Ge -3.0522910550 -5.4034609389 -1.0200302151
H -0.2566143279 2.7617791585 1.6800957653
H 0.4257500625 7.2134050943 1.8403189442
H 3.7812122058 6.7672490617 1.2145066734
H 4.4140583916 5.0725849142 4.0032599485
H 1.1692541843 5.2207232828 5.1614222016
H -2.7606700447 5.8033075402 3.9040632864
H -0.4760233355 7.3693545087 -1.7167627949
H 5.3616385158 5.2027813956 -1.3118359270
H 5.8179147923 2.0378876612 4.2155127286
H 0.9385752890 2.6283356637 7.3386258895
H -5.3622044837 5.1717673286 1.3248998641
H -3.8265398391 6.7688394867 -1.2128367918
H 0.2278559834 2.9402580308 -1.7144522173

H 2.9142637313 5.7787044685 -3.9720580930
H 3.1164598625 1.3980236016 -0.5663980065
H 7.3663051077 1.8135627620 0.8733687225
H 2.1937492176 0.0291651694 2.4445112971
H 3.2289388846 -0.0090687345 6.8415111820
H -2.0987783382 1.0535586230 7.1826324775
H -4.2612617670 3.2004131857 5.7610338337
H -3.0559567669 1.4035120466 0.5531202057
H -4.4520931510 5.0603214905 -3.9804711662
H -1.2742283630 5.1795354387 -5.3077152296
H 3.8585398167 2.8608198051 -5.9026986190
H 6.4505368993 1.6958958994 -3.5782607964
H 7.3229953754 -1.8369156519 0.8497710685
H 5.8010802976 -2.0220170683 4.2035893433
H 0.4065341279 -2.4193146344 7.1486796109
H -0.9566446333 -0.6874189155 3.2165449048
H -6.4056583817 1.7334508380 3.5331541438
H -7.3229953754 1.8369156519 -0.8497710685
H -5.8010802976 2.0220170683 -4.2035893433
H -0.4065341279 2.4193146344 -7.1486796109
H 0.9566446333 0.6874189155 -3.2165449048
H 6.4056583817 -1.7334508380 -3.5331541438
H 3.0559567669 -1.4035120466 -0.5531202057
H 4.4520931510 -5.0603214905 3.9804711662
H 1.2742283630 -5.1795354387 5.3077152296
H -3.8585398167 -2.8608198051 5.9026986190
H -6.4505368993 -1.6958958994 3.5782607964
H -7.3663051077 -1.8135627620 -0.8733687225
H -2.1937492176 -0.0291651694 -2.4445112971
H -3.2289388846 0.0090687345 -6.8415111820
H 2.0987783382 -1.0535586230 -7.1826324775
H 4.2612617670 -3.2004131857 -5.7610338337
H 5.3622044837 -5.1717673286 -1.3248998641
H 3.8265398391 -6.7688394867 1.2128367918
H -0.2278559834 -2.9402580308 1.7144522173
H -2.9142637313 -5.7787044685 3.9720580930
H -3.1164598625 -1.3980236016 0.5663980065
H -5.8179147923 -2.0378876612 -4.2155127286
H -0.9385752890 -2.6283356637 -7.3386258895
H 2.7606700447 -5.8033075402 -3.9040632864
H 0.4760233355 -7.3693545087 1.7167627949
H -5.3616385158 -5.2027813956 1.3118359270
H -4.4140583916 -5.0725849142 -4.0032599485
H -1.1692541843 -5.2207232828 -5.1614222016

H 0.2566143279 -2.7617791585 -1.6800957653
H -0.4257500625 -7.2134050943 -1.8403189442
H -3.7812122058 -6.7672490617 -1.2145066734

Isomer 5, HF =-124658.653118a.u.

Ge -0.4851966413 4.3238277709 2.6347237103
Ge 0.5549730946 5.9461513945 1.0843868162
Ge 2.9523542563 5.1935061355 1.0152241498
Ge 2.9370706421 3.2769664268 2.6012422535
Ge 1.2600105599 3.8566938936 4.3137008644
Ge -2.8448929507 4.5867758133 3.2328466503
Ge -0.6643816746 5.9676171369 -1.0636586431
Ge 4.0368875014 4.4551617898 -1.1033403752
Ge 4.9804127296 2.0406791298 3.1762708072
Ge 0.6852237861 2.0898285182 5.9371365217
Ge -4.1217571826 4.4613451998 1.0849066470
Ge -3.0992227475 5.3799585430 -1.0179489776
Ge 0.3044362196 4.2878528536 -2.5791106810
Ge 2.6825982251 4.4761940623 -3.1895867298
Ge 4.6074256980 2.0526340868 -0.9070848712
Ge 5.9751485506 1.2640043487 1.0023483508
Ge 4.2509983655 0.0198596106 4.4682729070
Ge 2.2195641548 0.0972854065 5.9232618770
Ge -1.6598540546 1.2498465399 5.6879771969
Ge -3.4907349454 2.6230493834 4.6736737297
Ge -4.5317070499 2.0311781610 1.0185011136
Ge -3.4789375475 3.9948773285 -3.1009122805
Ge -1.3477698822 3.9495395718 -4.3815460662
Ge 3.2906558775 2.4149858093 -4.4757401869
Ge 5.0775642414 1.2361644066 -3.2102155450
Ge 5.7214211029 -1.2037985922 0.9651838505
Ge 3.9750674803 -1.6286525140 2.6480148330
Ge 0.7122659667 -1.8736085891 5.6060271716
Ge -1.3286995824 -0.9237163483 4.5714577086
Ge -5.0794516516 1.2593680631 3.2934568814
Ge -5.7214211029 1.2037985922 -0.9651838505
Ge -3.9750674803 1.6286525140 -2.6480148330
Ge -0.7122659667 1.8736085891 -5.6060271716
Ge 1.3286995824 0.9237163483 -4.5714577086
Ge 5.0794516516 -1.2593680631 -3.2934568814
Ge 4.5317070499 -2.0311781610 -1.0185011136
Ge 3.4789375475 -3.9948773285 3.1009122805
Ge 1.3477698822 -3.9495395718 4.3815460662
Ge -3.2906558775 -2.4149858093 4.4757401869

Ge -5.0775642414 -1.2361644066 3.2102155450
Ge -5.9751485506 -1.2640043487 -1.0023483508
Ge -4.2509983655 -0.0198596106 -4.4682729070
Ge -2.2195641548 -0.0972854065 -5.9232618770
Ge 1.6598540546 -1.2498465399 -5.6879771969
Ge 3.4907349454 -2.6230493834 -4.6736737297
Ge 4.1217571826 -4.4613451998 -1.0849066470
Ge 3.0992227475 -5.3799585430 1.0179489776
Ge -0.3044362196 -4.2878528536 2.5791106810
Ge -2.6825982251 -4.4761940623 3.1895867298
Ge -4.6074256980 -2.0526340868 0.9070848712
Ge -4.9804127296 -2.0406791298 -3.1762708072
Ge -0.6852237861 -2.0898285182 -5.9371365217
Ge 2.8448929507 -4.5867758133 -3.2328466503
Ge 0.6643816746 -5.9676171369 1.0636586431
Ge -4.0368875014 -4.4551617898 1.1033403752
Ge -2.9370706421 -3.2769664268 -2.6012422535
Ge -1.2600105599 -3.8566938936 -4.3137008644
Ge 0.4851966413 -4.3238277709 -2.6347237103
Ge -0.5549730946 -5.9461513945 -1.0843868162
Ge -2.9523542563 -5.1935061355 -1.0152241498
H -0.5199022564 2.9993382019 1.8101148413
H 0.5247247902 7.3682378767 1.7148663572
H 3.8196517466 6.3466802029 1.5987706262
H 2.1623283939 2.1807412395 1.8059246207
H 1.6499791366 5.1524062697 5.0772586674
H -3.1176747005 5.9013433703 4.0151713381
H -0.5636974553 7.3799153887 -1.7099921731
H 5.3217195711 5.3084892608 -1.3070899243
H 6.0057552101 2.8839151032 3.9833301707
H 0.8219890072 2.7232305928 7.3536442269
H -5.4740499806 5.2149080781 1.2520702287
H -3.8725674582 6.7098618879 -1.2728319012
H 0.2329771587 2.9713422068 -1.7471036928
H 2.9439006983 5.7562183026 -4.0305334113
H 3.2183475515 1.4080608978 -0.6142038458
H 7.4580871911 1.7096215319 0.8765955023
H 5.4197001539 -0.4122304671 5.4023107377
H 2.7694199871 -0.0018961104 7.3783950700
H -2.1577095884 0.9510729867 7.1339408547
H -4.2963221582 3.1923751600 5.8800495235
H -3.1005126771 1.4472903017 0.8139472155
H -4.6210606182 4.6460946667 -3.9304288044
H -1.2859893835 5.1343841787 -5.3880199849

H 3.7574924730 2.7757491735 -5.9135770116
H 6.4739254043 1.7313454420 -3.6874692007
H 7.0430664014 -1.9648194038 1.2504169596
H 2.6870004180 -1.1242947763 1.9271102969
H 0.3163079659 -2.3290421731 7.0428746081
H -0.9744781021 -0.5947009081 3.0918787240
H -6.5195657935 1.7043847207 3.6827170672
H -7.0430664014 1.9648194038 -1.2504169596
H -2.6870004180 1.1242947763 -1.9271102969
H -0.3163079659 2.3290421731 -7.0428746081
H 0.9744781021 0.5947009081 -3.0918787240
H 6.5195657935 -1.7043847207 -3.6827170672
H 3.1005126771 -1.4472903017 -0.8139472155
H 4.6210606182 -4.6460946667 3.9304288044
H 1.2859893835 -5.1343841787 5.3880199849
H -3.7574924730 -2.7757491735 5.9135770116
H -6.4739254043 -1.7313454420 3.6874692007
H -7.4580871911 -1.7096215319 -0.8765955023
H -5.4197001539 0.4122304671 -5.4023107377
H -2.7694199871 0.0018961104 -7.3783950700
H 2.1577095884 -0.9510729867 -7.1339408547
H 4.2963221582 -3.1923751600 -5.8800495235
H 5.4740499806 -5.2149080781 -1.2520702287
H 3.8725674582 -6.7098618879 1.2728319012
H -0.2329771587 -2.9713422068 1.7471036928
H -2.9439006983 -5.7562183026 4.0305334113
H -3.2183475515 -1.4080608978 0.6142038458
H -6.0057552101 -2.8839151032 -3.9833301707
H -0.8219890072 -2.7232305928 -7.3536442269
H 3.1176747005 -5.9013433703 -4.0151713381
H 0.5636974553 -7.3799153887 1.7099921731
H -5.3217195711 -5.3084892608 1.3070899243
H -2.1623283939 -2.1807412395 -1.8059246207
H -1.6499791366 -5.1524062697 -5.0772586674
H 0.5199022564 -2.9993382019 -1.8101148413
H -0.5247247902 -7.3682378767 -1.7148663572
H -3.8196517466 -6.3466802029 -1.5987706262

Isomer 6, HF =-124658.6195351a.u.

Ge -2.0077138741 -0.6523457821 9.7269425306
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Ge 1.2408354139 1.7078634299 9.7269425306
Ge 2.0077138741 -0.6523457821 9.7269425306
Ge 0.0000000000 -2.1110352957 9.7269425306

Ge -3.2570703555 -1.0582863105 7.6162710546
Ge -2.0129801835 2.7706295308 7.6162710546
Ge 2.0129801835 2.7706295308 7.6162710546
Ge 3.2570703555 -1.0582863105 7.6162710546
Ge 0.0000000000 -3.4246864405 7.6162710546
Ge -3.4919175945 1.1345928041 6.4701681478
Ge 0.0000000000 3.6716194407 6.4701681478
Ge 3.4919175945 1.1345928041 6.4701681478
Ge 2.1581237593 -2.9704025244 6.4701681478
Ge -2.1581237593 -2.9704025244 6.4701681478
Ge -3.4919852573 1.1346147890 3.9814697916
Ge 0.0000000000 3.6716905856 3.9814697916
Ge 3.4919852573 1.1346147890 3.9814697916
Ge 2.1581655772 -2.9704600819 3.9814697916
Ge -2.1581655772 -2.9704600819 3.9814697916
Ge -2.1586454790 2.9711206100 2.9913851154
Ge 2.1586454790 2.9711206100 2.9913851154
Ge 3.4927617547 -1.1348670884 2.9913851154
Ge 0.0000000000 -3.6725070434 2.9913851154
Ge -3.4927617547 -1.1348670884 2.9913851154
Ge -2.1597296256 2.9726128098 0.4952384191
Ge 2.1597296256 2.9726128098 0.4952384191
Ge 3.4945159407 -1.1354370579 0.4952384191
Ge 0.0000000000 -3.6743515037 0.4952384191
Ge -3.4945159407 -1.1354370579 0.4952384191
Ge 0.0000000000 3.6743515037 -0.4952384191
Ge 3.4945159407 1.1354370579 -0.4952384191
Ge 2.1597296256 -2.9726128098 -0.4952384191
Ge -2.1597296256 -2.9726128098 -0.4952384191
Ge -3.4945159407 1.1354370579 -0.4952384191
Ge 0.0000000000 3.6725070434 -2.9913851154
Ge 3.4927617547 1.1348670884 -2.9913851154
Ge 2.1586454790 -2.9711206100 -2.9913851154
Ge -2.1586454790 -2.9711206100 -2.9913851154
Ge -3.4927617547 1.1348670884 -2.9913851154
Ge 2.1581655772 2.9704600819 -3.9814697916
Ge 3.4919852573 -1.1346147890 -3.9814697916
Ge 0.0000000000 -3.6716905856 -3.9814697916
Ge -3.4919852573 -1.1346147890 -3.9814697916
Ge -2.1581655772 2.9704600819 -3.9814697916
Ge 2.1581237593 2.9704025244 -6.4701681478
Ge 3.4919175945 -1.1345928041 -6.4701681478
Ge 0.0000000000 -3.6716194407 -6.4701681478
Ge -3.4919175945 -1.1345928041 -6.4701681478

Ge -2.1581237593 2.9704025244 -6.4701681478
Ge 3.2570703555 1.0582863105 -7.6162710546
Ge 2.0129801835 -2.7706295308 -7.6162710546
Ge -2.0129801835 -2.7706295308 -7.6162710546
Ge -3.2570703555 1.0582863105 -7.6162710546
Ge 0.0000000000 3.4246864405 -7.6162710546
Ge 2.0077138741 0.6523457821 -9.7269425306
Ge 1.2408354139 -1.7078634299 -9.7269425306
Ge -1.2408354139 -1.7078634299 -9.7269425306
Ge -2.0077138741 0.6523457821 -9.7269425306
Ge 0.0000000000 2.1110352957 -9.7269425306
H -2.9067774865 -0.9444692579 10.9587069174
H -1.7964872844 2.4726526186 10.9587069174
H 1.7964872844 2.4726526186 10.9587069174
H 2.9067774865 -0.9444692579 10.9587069174
H 0.0000000000 -3.0563667213 10.9587069174
H -4.7005973281 -1.5273166559 7.9570497922
H -2.9051289162 3.9985669169 7.9570497922
H 2.9051289162 3.9985669169 7.9570497922
H 4.7005973281 -1.5273166559 7.9570497922
H 0.0000000000 -4.9425005218 7.9570497922
H -4.9275437600 1.6010560217 6.8586532829
H 0.0000000000 5.1811261220 6.8586532829
H 4.9275437600 1.6010560217 6.8586532829
H 3.0453895248 -4.1916190827 6.8586532829
H -3.0453895248 -4.1916190827 6.8586532829
H -4.9345622961 1.6033364823 3.6142952366
H 0.0000000000 5.1885058475 3.6142952366
H 4.9345622961 1.6033364823 3.6142952366
H 3.0497272186 -4.1975894061 3.6142952366
H -3.0497272186 -4.1975894061 3.6142952366
H -3.0502217296 4.1982700420 3.3613131496
H 3.0502217296 4.1982700420 3.3613131496
H 4.9353624316 -1.6035964621 3.3613131496
H 0.0000000000 -5.1893471598 3.3613131496
H -4.9353624316 -1.6035964621 3.3613131496
H -3.0516990602 4.2003034132 0.1299672027
H 3.0516990602 4.2003034132 0.1299672027
H 4.9377528029 -1.6043731408 0.1299672027
H 0.0000000000 -5.1918605449 0.1299672027
H -4.9377528029 -1.6043731408 0.1299672027
H 0.0000000000 5.1918605449 -0.1299672027
H 4.9377528029 1.6043731408 -0.1299672027
H 3.0516990602 -4.2003034132 -0.1299672027

H -3.0516990602 -4.2003034132 -0.1299672027
H -4.9377528029 1.6043731408 -0.1299672027
H 0.0000000000 5.1893471598 -3.3613131496
H 4.9353624316 1.6035964621 -3.3613131496
H 3.0502217296 -4.1982700420 -3.3613131496
H -3.0502217296 -4.1982700420 -3.3613131496
H -4.9353624316 1.6035964621 -3.3613131496
H 3.0497272186 4.1975894061 -3.6142952366
H 4.9345622961 -1.6033364823 -3.6142952366
H 0.0000000000 -5.1885058475 -3.6142952366
H -4.9345622961 -1.6033364823 -3.6142952366
H -3.0497272186 4.1975894061 -3.6142952366
H 3.0453895248 4.1916190827 -6.8586532829
H 4.9275437600 -1.6010560217 -6.8586532829
H 0.0000000000 -5.1811261220 -6.8586532829
H -4.9275437600 -1.6010560217 -6.8586532829
H -3.0453895248 4.1916190827 -6.8586532829
H 4.7005973281 1.5273166559 -7.9570497922
H 2.9051289162 -3.9985669169 -7.9570497922
H -2.9051289162 -3.9985669169 -7.9570497922
H -4.7005973281 1.5273166559 -7.9570497922
H 0.0000000000 4.9425005218 -7.9570497922
H 2.9067774865 0.9444692579 -10.9587069174
H 1.7964872844 -2.4726526186 -10.9587069174
H -1.7964872844 -2.4726526186 -10.9587069174
H -2.9067774865 0.9444692579 -10.9587069174
H 0.0000000000 3.0563667213 -10.9587069174

Isomer 7, HF =-124658.6430389a.u.

Ge -0.7167664646 9.7094212994 2.0073834441
Ge -2.1763768620 9.6618066370 0.0000000000
Ge -0.7167664646 9.7094212994 -2.0073834441
Ge 1.6433434468 9.7061167881 -1.2405913984
Ge 1.6433434468 9.7061167881 1.2405913984
Ge -1.1024065636 7.6167935326 3.2891892354
Ge -3.4321444620 7.5127514549 0.0000000000
Ge -1.1024065636 7.6167935326 -3.2891892354
Ge 2.7030120866 7.5955495361 -2.0191823390
Ge 2.7030120866 7.5955495361 2.0191823390
Ge -2.9414861905 6.3871526950 2.1663789283
Ge -2.9414861905 6.3871526950 -2.1663789283
Ge 1.0947661428 6.4892067805 -3.5618834322
Ge 3.5549201953 6.4225165477 0.0000000000
Ge 1.0947661428 6.4892067805 3.5618834322

Ge -2.7168035197 3.9207311907 2.1287862659
Ge -2.7168035197 3.9207311907 -2.1287862659
Ge 1.1067359412 3.9979789642 -3.6682362271
Ge 3.4704664817 3.9381952431 0.0000000000
Ge 1.1067359412 3.9979789642 3.6682362271
Ge -2.0467274647 2.8870726710 0.0000000000
Ge -1.1552726406 2.9914954094 -3.8045479889
Ge 2.8202098848 2.9780424186 -2.1940501184
Ge 2.8202098848 2.9780424186 2.1940501184
Ge -1.1552726406 2.9914954094 3.8045479889
Ge -3.0724750397 0.6417453718 0.0000000000
Ge -1.1399578774 0.4856514453 -3.7616373221
Ge 2.8061011503 0.4870680306 -2.1984003930
Ge 2.8061011503 0.4870680306 2.1984003930
Ge -1.1399578774 0.4856514453 3.7616373221
Ge -2.8061011503 -0.4870680306 -2.1984003930
Ge 1.1399578774 -0.4856514453 -3.7616373221
Ge 3.0724750397 -0.6417453718 0.0000000000
Ge 1.1399578774 -0.4856514453 3.7616373221
Ge -2.8061011503 -0.4870680306 2.1984003930
Ge -2.8202098848 -2.9780424186 -2.1940501184
Ge 1.1552726406 -2.9914954094 -3.8045479889
Ge 2.0467274647 -2.8870726710 0.0000000000
Ge 1.1552726406 -2.9914954094 3.8045479889
Ge -2.8202098848 -2.9780424186 2.1940501184
Ge -1.1067359412 -3.9979789642 -3.6682362271
Ge 2.7168035197 -3.9207311907 -2.1287862659
Ge 2.7168035197 -3.9207311907 2.1287862659
Ge -1.1067359412 -3.9979789642 3.6682362271
Ge -3.4704664817 -3.9381952431 0.0000000000
Ge -1.0947661428 -6.4892067805 -3.5618834322
Ge 2.9414861905 -6.3871526950 -2.1663789283
Ge 2.9414861905 -6.3871526950 2.1663789283
Ge -1.0947661428 -6.4892067805 3.5618834322
Ge -3.5549201953 -6.4225165477 0.0000000000
Ge 1.1024065636 -7.6167935326 -3.2891892354
Ge 3.4321444620 -7.5127514549 0.0000000000
Ge 1.1024065636 -7.6167935326 3.2891892354
Ge -2.7030120866 -7.5955495361 2.0191823390
Ge -2.7030120866 -7.5955495361 -2.0191823390
Ge 0.7167664646 -9.7094212994 -2.0073834441
Ge 2.1763768620 -9.6618066370 0.0000000000
Ge 0.7167664646 -9.7094212994 2.0073834441
Ge -1.6433434468 -9.7061167881 1.2405913984

Ge -1.6433434468 -9.7061167881 -1.2405913984
H -1.0144780567 10.9555599118 2.8851636196
H -3.1617294500 10.8624713464 0.0000000000
H -1.0144780567 10.9555599118 -2.8851636196
H 2.4071170516 10.9389203197 -1.7955421656
H 2.4071170516 10.9389203197 1.7955421656
H -1.6122450992 7.9631691841 4.7167369345
H -4.9580060169 7.8159223137 0.0000000000
H -1.6122450992 7.9631691841 -4.7167369345
H 3.9563001894 7.9418799491 -2.8735920021
H 3.9563001894 7.9418799491 2.8735920021
H -4.1993836713 6.6609322441 3.0439268427
H -4.1993836713 6.6609322441 -3.0439268427
H 1.5719713426 6.9444968762 -4.9741999243
H 5.0765870081 6.7596932937 0.0000000000
H 1.5719713426 6.9444968762 4.9741999243
H -4.1337312523 3.3566950889 2.4380574251
H -4.1337312523 3.3566950889 -2.4380574251
H 1.7138967497 3.6890081796 -5.0712763077
H 4.9803067179 3.5371675299 0.0000000000
H 1.7138967497 3.6890081796 5.0712763077
H -0.4900559670 2.7639414821 0.0000000000
H -1.6674798700 3.3971324443 -5.2197148080
H 4.1120315850 3.3209163372 -3.0027025578
H 4.1120315850 3.3209163372 3.0027025578
H -1.6674798700 3.3971324443 5.2197148080
H -4.5966165558 0.9700064193 0.0000000000
H -1.7035171563 0.0658433543 -5.1544726371
H 4.1529922841 0.1157357379 -2.8905243039
H 4.1529922841 0.1157357379 2.8905243039
H -1.7035171563 0.0658433543 5.1544726371
H -4.1529922841 -0.1157357379 -2.8905243039
H 1.7035171563 -0.0658433543 -5.1544726371
H 4.5966165558 -0.9700064193 0.0000000000
H 1.7035171563 -0.0658433543 5.1544726371
H -4.1529922841 -0.1157357379 2.8905243039
H -4.1120315850 -3.3209163372 -3.0027025578
H 1.6674798700 -3.3971324443 -5.2197148080
H 0.4900559670 -2.7639414821 0.0000000000
H 1.6674798700 -3.3971324443 5.2197148080
H -4.1120315850 -3.3209163372 3.0027025578
H -1.7138967497 -3.6890081796 -5.0712763077
H 4.1337312523 -3.3566950889 -2.4380574251
H 4.1337312523 -3.3566950889 2.4380574251

H -1.7138967497 -3.6890081796 5.0712763077
H -4.9803067179 -3.5371675299 0.0000000000
H -1.5719713426 -6.9444968762 -4.9741999243
H 4.1993836713 -6.6609322441 -3.0439268427
H 4.1993836713 -6.6609322441 3.0439268427
H -1.5719713426 -6.9444968762 4.9741999243
H -5.0765870081 -6.7596932937 0.0000000000
H 1.6122450992 -7.9631691841 -4.7167369345
H 4.9580060169 -7.8159223137 0.0000000000
H 1.6122450992 -7.9631691841 4.7167369345
H -3.9563001894 -7.9418799491 2.8735920021
H -3.9563001894 -7.9418799491 -2.8735920021
H 1.0144780567 -10.9555599118 -2.8851636196
H 3.1617294500 -10.8624713464 0.0000000000
H 1.0144780567 -10.9555599118 2.8851636196
H -2.4071170516 -10.9389203197 1.7955421656
H -2.4071170516 -10.9389203197 -1.7955421656

Isomer 8, HF =-124658.6625892a.u.

Ge 2.1112711195 9.6596101367 0.0000000000
Ge 0.6530995770 9.7005112326 2.0088264701
Ge -1.7061911927 9.6831542503 1.2423389850
Ge -1.7061911927 9.6831542503 -1.2423389850
Ge 0.6530995770 9.7005112326 -2.0088264701
Ge 3.3673174927 7.5129838770 0.0000000000
Ge 1.0461159081 7.6135008698 3.3006745961
Ge -2.7512547015 7.5681547223 2.0279239625
Ge -2.7512547015 7.5681547223 -2.0279239625
Ge 1.0461159081 7.6135008698 -3.3006745961
Ge 2.8757822428 6.3820522931 2.1601437377
Ge -1.1529364098 6.4975575972 3.6231546235
Ge -3.3606600543 6.2689226206 0.0000000000
Ge -1.1529364098 6.4975575972 -3.6231546235
Ge 2.8757822428 6.3820522931 -2.1601437377
Ge 2.6804772554 3.9122149946 2.1349041470
Ge -1.1408025394 3.9997009733 3.8127225034
Ge -2.2092514494 4.1012626612 0.0000000000
Ge -1.1408025394 3.9997009733 -3.8127225034
Ge 2.6804772554 3.9122149946 -2.1349041470
Ge 1.1357363442 2.9963336537 3.8373934055
Ge -2.6809328071 2.9965417453 2.1540985427
Ge -2.6809328071 2.9965417453 -2.1540985427
Ge 1.1357363442 2.9963336537 -3.8373934055
Ge 2.1369379759 2.8041500359 0.0000000000

Ge 1.1372162404 0.4903935986 3.7355088160
Ge -2.8159052827 0.5148415104 2.1953625184
Ge -2.8159052827 0.5148415104 -2.1953625184
Ge 1.1372162404 0.4903935986 -3.7355088160
Ge 3.2138363976 0.5904667682 0.0000000000
Ge -1.1372162404 -0.4903935986 3.7355088160
Ge -3.2138363976 -0.5904667682 0.0000000000
Ge -1.1372162404 -0.4903935986 -3.7355088160
Ge 2.8159052827 -0.5148415104 -2.1953625184
Ge 2.8159052827 -0.5148415104 2.1953625184
Ge -1.1357363442 -2.9963336537 3.8373934055
Ge -2.1369379759 -2.8041500359 0.0000000000
Ge -1.1357363442 -2.9963336537 -3.8373934055
Ge 2.6809328071 -2.9965417453 -2.1540985427
Ge 2.6809328071 -2.9965417453 2.1540985427
Ge -2.6804772554 -3.9122149946 2.1349041470
Ge -2.6804772554 -3.9122149946 -2.1349041470
Ge 1.1408025394 -3.9997009733 -3.8127225034
Ge 2.2092514494 -4.1012626612 0.0000000000
Ge 1.1408025394 -3.9997009733 3.8127225034
Ge -2.8757822428 -6.3820522931 2.1601437377
Ge -2.8757822428 -6.3820522931 -2.1601437377
Ge 1.1529364098 -6.4975575972 -3.6231546235
Ge 3.3606600543 -6.2689226206 0.0000000000
Ge 1.1529364098 -6.4975575972 3.6231546235
Ge -3.3673174927 -7.5129838770 0.0000000000
Ge -1.0461159081 -7.6135008698 -3.3006745961
Ge 2.7512547015 -7.5681547223 -2.0279239625
Ge 2.7512547015 -7.5681547223 2.0279239625
Ge -1.0461159081 -7.6135008698 3.3006745961
Ge -2.1112711195 -9.6596101367 0.0000000000
Ge -0.6530995770 -9.7005112326 -2.0088264701
Ge 1.7061911927 -9.6831542503 -1.2423389850
Ge 1.7061911927 -9.6831542503 1.2423389850
Ge -0.6530995770 -9.7005112326 2.0088264701
H 3.0950285508 10.8616511256 0.0000000000
H 0.9438342338 10.9511157409 2.8828436701
H -2.4763883240 10.9135497989 1.7943751438
H -2.4763883240 10.9135497989 -1.7943751438
H 0.9438342338 10.9511157409 -2.8828436701
H 4.8935465662 7.8142103193 0.0000000000
H 1.5841608997 7.9741851607 4.7146583568
H -4.0515739633 7.8894088041 2.8187632375
H -4.0515739633 7.8894088041 -2.8187632375

H 1.5841608997 7.9741851607 -4.7146583568
H 4.1340646143 6.6589290025 3.0368340420
H -1.6239989413 6.9979457093 5.0229416411
H -4.8977314595 6.0396818677 0.0000000000
H -1.6239989413 6.9979457093 -5.0229416411
H 4.1340646143 6.6589290025 -3.0368340420
H 4.0986800507 3.3877967314 2.5082116935
H -1.7298145434 3.6896628156 5.2217467616
H -0.6991648555 4.4842123832 0.0000000000
H -1.7298145434 3.6896628156 -5.2217467616
H 4.0986800507 3.3877967314 -2.5082116935
H 1.7241541828 3.3642259961 5.2330634538
H -4.1088962926 3.4830237209 2.5440595962
H -4.1088962926 3.4830237209 -2.5440595962
H 1.7241541828 3.3642259961 -5.2330634538
H 0.6108053985 2.5005788214 0.0000000000
H 1.6957456242 0.0459740095 5.1237978650
H -4.1539700760 0.2358525217 2.9463932949
H -4.1539700760 0.2358525217 -2.9463932949
H 1.6957456242 0.0459740095 -5.1237978650
H 4.7526601221 0.8293963875 0.0000000000
H -1.6957456242 -0.0459740095 5.1237978650
H -4.7526601221 -0.8293963875 0.0000000000
H -1.6957456242 -0.0459740095 -5.1237978650
H 4.1539700760 -0.2358525217 -2.9463932949
H 4.1539700760 -0.2358525217 2.9463932949
H -1.7241541828 -3.3642259961 5.2330634538
H -0.6108053985 -2.5005788214 0.0000000000
H -1.7241541828 -3.3642259961 -5.2330634538
H 4.1088962926 -3.4830237209 -2.5440595962
H 4.1088962926 -3.4830237209 2.5440595962
H -4.0986800507 -3.3877967314 2.5082116935
H -4.0986800507 -3.3877967314 -2.5082116935
H 1.7298145434 -3.6896628156 -5.2217467616
H 0.6991648555 -4.4842123832 0.0000000000
H 1.7298145434 -3.6896628156 5.2217467616
H -4.1340646143 -6.6589290025 3.0368340420
H -4.1340646143 -6.6589290025 -3.0368340420
H 1.6239989413 -6.9979457093 -5.0229416411
H 4.8977314595 -6.0396818677 0.0000000000
H 1.6239989413 -6.9979457093 5.0229416411
H -4.8935465662 -7.8142103193 0.0000000000
H -1.5841608997 -7.9741851607 -4.7146583568
H 4.0515739633 -7.8894088041 -2.8187632375

H 4.0515739633 -7.8894088041 2.8187632375
H -1.5841608997 -7.9741851607 4.7146583568
H -3.0950285508 -10.8616511256 0.0000000000
H -0.9438342338 -10.9511157409 -2.8828436701
H 2.4763883240 -10.9135497989 -1.7943751438
H 2.4763883240 -10.9135497989 1.7943751438
H -0.9438342338 -10.9511157409 2.8828436701

Isomer 9, HF=-124658.666246a.u.

Ge 2.0556236831 9.6851056029 0.0000000000
Ge 0.5950240971 9.6808930332 2.0059576991
Ge -1.7689955971 9.6504961934 1.2395212567
Ge -1.7689955971 9.6504961934 -1.2395212567
Ge 0.5950240971 9.6808930332 -2.0059576991
Ge 3.3886050496 7.5816102230 0.0000000000
Ge 1.0259015304 7.5814320216 3.2615824303
Ge -2.8200740718 7.5315598032 2.0085916614
Ge -2.8200740718 7.5315598032 -2.0085916614
Ge 1.0259015304 7.5814320216 -3.2615824303
Ge 2.9707132880 6.4541603419 2.1820640528
Ge -1.0993493163 6.3013577134 3.3145110277
Ge -3.7812563670 6.3981148446 0.0000000000
Ge -1.0993493163 6.3013577134 -3.3145110277
Ge 2.9707132880 6.4541603419 -2.1820640528
Ge 3.0881524024 3.9580574260 2.2183280566
Ge -0.7384297224 4.0437880197 2.4177138011
Ge -3.8929142213 3.8882187536 0.0000000000
Ge -0.7384297224 4.0437880197 -2.4177138011
Ge 3.0881524024 3.9580574260 -2.2183280566
Ge 1.1929494790 2.9746306666 3.5187191510
Ge -2.9058487002 2.9305767051 2.0742701413
Ge -2.9058487002 2.9305767051 -2.0742701413
Ge 1.1929494790 2.9746306666 -3.5187191510
Ge 3.4482138347 2.8655540298 0.0000000000
Ge 1.1538035553 0.4816851669 3.7565030825
Ge -2.7718117613 0.4600074846 2.1299821433
Ge -2.7718117613 0.4600074846 -2.1299821433
Ge 1.1538035553 0.4816851669 -3.7565030825
Ge 2.2968390984 0.6843389428 0.0000000000
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Ge 2.7718117613 -0.4600074846 -2.1299821433
Ge 2.7718117613 -0.4600074846 2.1299821433

Ge -1.1929494790 -2.9746306666 3.5187191510
Ge -3.4482138347 -2.8655540298 0.0000000000
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Ge 2.9058487002 -2.9305767051 -2.0742701413
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Ge -3.0881524024 -3.9580574260 2.2183280566
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Ge 0.7384297224 -4.0437880197 -2.4177138011
Ge 3.8929142213 -3.8882187536 0.0000000000
Ge 0.7384297224 -4.0437880197 2.4177138011
Ge -2.9707132880 -6.4541603419 2.1820640528
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Ge 1.0993493163 -6.3013577134 -3.3145110277
Ge 3.7812563670 -6.3981148446 0.0000000000
Ge 1.0993493163 -6.3013577134 3.3145110277
Ge -3.3886050496 -7.5816102230 0.0000000000
Ge -1.0259015304 -7.5814320216 -3.2615824303
Ge 2.8200740718 -7.5315598032 -2.0085916614
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Ge -1.0259015304 -7.5814320216 3.2615824303
Ge -2.0556236831 -9.6851056029 0.0000000000
Ge -0.5950240971 -9.6808930332 -2.0059576991
Ge 1.7689955971 -9.6504961934 -1.2395212567
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H 2.9924063211 10.9247466761 0.0000000000
H 0.8679309550 10.9213485167 2.9000153184
H -2.5442155420 10.8768181766 1.7939608781
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H -4.0064603827 7.8565964487 2.9608262373
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H 1.4432094805 7.9157954309 -4.7221478992
H 4.1849078749 6.9054406137 3.0512729618
H -1.5848308416 6.2057656209 4.7883859129
H -5.2753839939 6.8469561169 0.0000000000
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H 4.1849078749 6.9054406137 -3.0512729618
H 4.4063707685 3.6408168353 2.9884995927
H -0.2024374068 4.3029902245 0.9802357323
H -5.4103984648 3.5304829483 0.0000000000
H -0.2024374068 4.3029902245 -0.9802357323

H 4.4063707685 3.6408168353 -2.9884995927
H 1.2915499561 3.5521253317 4.9621715357
H -3.8340833771 3.3388887953 3.2562221807
H -3.8340833771 3.3388887953 -3.2562221807
H 1.2915499561 3.5521253317 -4.9621715357
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H 0.7713749888 1.0003290019 0.0000000000
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H 4.0064603827 -7.8565964487 2.9608262373
H -1.4432094805 -7.9157954309 4.7221478992
H -2.9924063211 -10.9247466761 0.0000000000
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Isomer 10, HF =-124658.6630652a.u.

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Ge 9.6913650000 -0.6757300000 -1.9755260000
Ge 9.6977330000 -2.1392930000 0.0325110000
Ge 9.7067370000 -0.6822350000 2.0399870000
Ge 9.7450190000 1.6799160000 1.2719990000
Ge 7.5923150000 2.7663890000 -1.9571810000
Ge 7.5711880000 -1.0696040000 -3.2100450000
Ge 7.5869700000 -3.4526780000 0.0470550000
Ge 7.5908770000 -1.0678500000 3.2948530000
Ge 7.6737450000 2.7856000000 2.0826820000
Ge 6.4292930000 1.1356680000 -3.4467500000
Ge 6.3321220000 -2.8608140000 -2.0140300000
Ge 6.4533600000 -3.0283440000 2.2295930000
Ge 6.4093530000 1.1220280000 3.4299710000
Ge 6.5181090000 3.7236650000 0.0794960000
Ge 3.9336590000 1.1645440000 -3.4432320000
Ge 4.0563190000 -2.1245320000 -1.4522060000
Ge 3.9471760000 -3.1474920000 2.2889790000
Ge 4.1461080000 0.9259210000 2.5022010000
Ge 4.0287330000 3.8142960000 0.0694290000
Ge 2.9400000000 -1.1235190000 -3.4118540000
Ge 2.9825420000 -3.7538320000 0.0619230000
Ge 2.8990160000 -1.0824580000 3.2048490000
Ge 3.0096940000 3.1291250000 2.2363540000
Ge 2.9064870000 2.2258640000 -1.4585350000
Ge 0.4526930000 -1.1651310000 -3.3091770000
Ge 0.4865910000 -3.9369220000 -0.0583720000
Ge 0.6499200000 -0.7815520000 2.2559000000
Ge 0.4913750000 3.2168160000 2.2493170000
Ge 0.5825930000 2.8860460000 -1.9170950000
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Ge -2.9400000000 1.1235190000 3.4118540000
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H 2.8366610000 -1.1925480000 4.7534490000
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Ge 2.4419033768 -0.6795273800 9.2166693880
Ge 2.4894324923 0.7275094973 11.2654517502
Ge 0.7275094973 2.4894324923 11.2654517502
Ge 0.6795273800 -2.4419033768 9.2166693880
Ge -0.7024996640 -2.4590796703 7.1572920564
Ge 0.7021504405 -2.4594598019 5.1141103989
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Ge -2.4590796703 -0.7024996640 7.1572920564

Ge -2.4419033768 0.6795273800 9.2166693880
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Ge 2.4582985408 -0.7008904637 1.0228173795
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Ge -0.7008904637 2.4582985408 1.0228173795
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Ge 2.4582985408 0.7008904637 -1.0228173795
Ge -2.4582985408 0.7008904637 1.0228173795
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Ge 2.4580662240 -0.7004913731 -3.0687637179
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Ge -0.7024996640 2.4590796703 -7.1572920564
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Ge -2.5821146661 -0.8242478813 -13.1825931650
Ge -0.8242478813 -2.5821146661 -13.1825931650
Ge -0.7275094973 2.4894324923 -11.2654517502
Ge 0.8242478813 2.5821146661 -13.1825931650
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Ge -0.8639974568 0.8639974568 14.9696021524
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H 3.8146036112 -1.4679123930 1.0227478172
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H -1.3361853386 1.3361853386 16.3698235069
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Isomer 11, HF =-124658.5931734a.u.

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Ge -2.2146787512 1.2454114603 8.1919769052
Ge -1.2417098947 2.2836863909 10.2285466859
Ge -2.3295038110 1.2503784748 12.1979242730
Ge -2.3295038110 -1.2503784748 12.1979242730
Ge 1.2417098947 2.2836863909 10.2285466859
Ge 2.2146787512 1.2454114603 8.1919769052
Ge 1.2424256258 2.2325070036 6.1351240147
Ge -1.2424256258 2.2325070036 6.1351240147
Ge 2.2146787512 -1.2454114603 8.1919769052
Ge 1.2417098947 -2.2836863909 10.2285466859
Ge 2.3295038110 -1.2503784748 12.1979242730
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Ge 1.2424256258 -2.2325070036 6.1351240147
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Ge -2.2363855774 -1.2424166797 4.0906024203
Ge -2.2363855774 1.2424166797 4.0906024203
Ge -1.2428023736 2.2336427220 2.0458619122
Ge 1.2428023736 2.2336427220 2.0458619122

Ge 2.2363855774 1.2424166797 4.0906024203
Ge 2.2363855774 -1.2424166797 4.0906024203
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